

Calculation of Upper Limit of Hydrogens of an Organic Formula for Analysis of Mass Spectra

SIR: In developing computer programs (3) for the analysis of mass spectral data, it became desirable to calculate the maximum number of hydrogen atoms (hydrogen value, HV) which a molecule of given integer molecular weight (W) may contain.

A formula has been developed which requires only the use of integer arithmetic. A parameter (x) may be calculated which is related to the integer residue (r) obtained on dividing the molecular weight (W) by 14. The upper limit of hydrogens (HV) for a given molecular weight (W) is then given by the expression:

$$HV = 2(W/14) + x \quad (1)$$

in which the value of x is determined by the residue and obtained from Table I.

Only the integer portion of ($W/14$) is utilized in Equation 1.

To illustrate the necessary procedure, a few examples have been incorporated in the right hand portion of Table I.

If the molecular weight of a compound is 148, then the appropriate values of r and x are 8 and -4 (See Table I).

Bearing in mind that only the integer portion of $W/14$ is utilized, we have

$$\begin{aligned} HV &= 2(148/14) + (-4) \\ &= 2(10) - 4 \\ &= 20 - 4 = 16 \end{aligned}$$

The formula $C_4H_{16}N_6$ is given as a possibility in Table I; however, other combinations of C, N, and O can give

Table I. Values of Parameter (x) and Maximum Hydrogen Values for Sample Molecular Weights

Re- mainder (r)	Examples			
	x	w	HV	Possible formula
0	0	140	20	$C_{10}H_{20}$
1	-1	141	19	$C_9H_{19}N$
2	2	142	22	$C_{10}H_{22}$
3	1	143	21	$C_9H_{21}N$
4	0	144	20	$C_8H_{20}N_2$
5	-1	145	19	$C_7H_{19}N_3$
6	-2	146	18	$C_6H_{18}N_4$
7	-3	147	17	$C_5H_{17}N_5$
8	-4	148	16	$C_4H_{16}N_6$
9	-5	149	15	$C_{10}H_{15}N$
10	-2	150	18	$C_{11}H_{18}$
11	-3	151	17	$C_{10}H_{17}N$
12	0	152	20	$C_{11}H_{20}$
13	-1	153	19	$C_{10}H_{19}N$
0	0	154	22	$C_{11}H_{22}$

alternatives with the same hydrogen value—e.g., $C_{11}H_{16}$ or $C_6H_{16}N_2O_2$.

The above procedure is applicable to intact organic molecules of any level of saturation containing C^{12} , H^1 , N^{14} , or O^{16} . Other species—e.g., radicals or isotopic substitutions—should be revised to the corresponding standard forms by adding or subtracting the appropriate weights before the calculation is applied.

The arithmetic basis of these calculations—almost self-evident from the valence rules and the fact of CH_2 weighing 14—is elaborated elsewhere (1-4).

LITERATURE CITED

- (1) Lederberg, J., "Computation of Molecular Formulas for Mass Spectrometry," Holden-Day, Inc., San Francisco, 1964.
- (2) Lederberg, J., NASA STAR N64-21426, 1964.
- (3) Lederberg, J., Wightman, M., "A Subalgol Program for Calculation of Molecular Compositional Formulas from Mass Spectral Data," Rept. to NASA, Grant No. 81-60, 1964.
- (4) Kendrick, E., ANAL. CHEM. **35**, 2146 (1963).

JOSHUA LEDERBERG
MARGARET WIGHTMAN

Stanford University School of Medicine
Palo Alto, Calif.

A reprint from

**ANALYTICAL
CHEMISTRY**

Vol. 36, November 1964, Pages 2365
Copyright 1964 by the American Chemical
Society and reprinted by permission of
the copyright owner